

# Assessment of CEX ion backflow of SPT-100 thruster

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**Abstract.** The SPT-100 thruster plume was simulated using two different methods: the combined particle-in-cell technique with direct simulation Monte Carlo method and the particle-in-cell with the addition of Monte Carlo collisions method. The former method offers a more detailed description of the plume, taking into account the effect of ion-neutral collisions on neutral flow. This effect is ignored in the second method, but this method has much lower computational cost. To analyze the influence of uncertainties in plasma parameters at the thruster exit plane, the computations with different boundary conditions were performed. It is shown that the difference in results obtained by the two methods is significantly smaller than that caused by the uncertainty in flow parameters at the thruster exit plane.

## INTRODUCTION

One of the main problems of Stationary Plasma Thrusters (SPT) application for propulsion purposes is the accurate prediction of contamination of the sensitive surfaces of the spacecraft. There are two major sources of contamination: direct impingement of fast propellant ions onto the surfaces and backflow current of slow ions caused by formation of a charge exchange (CEX) plasma. The fast ion flow in the core of the plume can be described even by a simple semi-empirical model very effectively (see, for example, [1]). A much more detailed analysis of the SPT plume is required to predict the backflow current. In this case, some part of fast ions of the SPT plasma plume is scattered on neutral atoms of the propellant, which leads to appearance of slow ions. Under the action of an electric field, these ions move backwards and create the backflow current. The magnitude of this current should be correctly estimated to predict the level of contamination of the spacecraft surfaces.

The drawback of experimental investigation of the plasma surrounding the thruster is the impossibility of creating actual space conditions in ground-based facilities, since it is not possible to reach hard vacuum in a test chamber, and hence, an ambient gas is present there. It is known that the ambient gas has a considerable effect on the magnitude of the backflow current [2]. Therefore, extrapolation of experimental data to actual space conditions requires numerical simulation of the SPT thruster plume.

The combined the particle-in-cell technique with the direct simulation Monte Carlo (PIC-DSMC) method was used for simulation of SPT thruster plume flows in [2,3], which takes into account only ion-neutral collisions. However, application of this method for computing of the SPT thruster plume flows with taking into account ambient gas requires large computer resources. The reason is that the number density of the ambient gas is usually comparable with the density of the propellant neutrals at the thruster exit plane. Therefore, the number of model particles for the ambient gas is orders of magnitude greater than the number of model particles for ions and propellant neutrals. To overcome this difficulty, it was proposed in [3,4] to consider the ambient gas as separate species with constant parameters.

In this aspect, it seems of interest to use the classic particle-in-cell with the addition of Monte Carlo collisions (PIC-MCC) method [5] for simulation of ions in SPT thruster plume. The DSMC method is preliminary used to calculate the propellant neutral plume taking into account the ambient gas. This approach also takes into account ion-neutral collisions, but in contrast to the PIC-DSMC method, the change in the neutral flow due to these collisions is ignored.

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The main goals of the paper are the comparison of PIC-MCC and PIC-DSMC methods for modeling of plasma plume flows exhausted from SPT-100 and the study of the influence of thruster exit plane conditions on the CEX ion backflow.

## PHYSICAL MODEL OF THE THRUSTER PLUME

Plasma surrounding the thruster is a multispecies medium, which consists of:

1. fast propellant  $Xe^+$  and  $Xe^{++}$  ions with the energy of directed motion of about 300 eV and density of about  $10^{17} \text{ \#}/m^3$ ,
2. neutrals of un-ionized Xenon propellant (temperature  $\sim 1000 \text{ K}$ , and density of about  $10^{18} \text{ \#}/m^3$ ), exhausted from thruster with thermal velocities,
3. slow  $Xe^+$  and  $Xe^{++}$  ions, which appear in the course of scattering of fast ions on neutral atoms,
4. electrons (temperature  $\sim 1 - 10 \text{ eV}$ ) emitted by the hollow cathode, and
5. ions and neutrals of various kinds obtained by sputtering from the surface of the thruster channel walls.

All the above-mentioned components interact with each other by means of the following processes: Coulomb interaction of charged particles, CEX collisions of ions with neutrals, elastic collisions of charged particles with neutrals, ionization and excitation of neutrals by an electron-neutral collisions. In addition, charged components of the plume interact with a self-consistent electric field  $\vec{E}$  arising because of separation of charges in the plasma and with a magnetic field  $\vec{B}$  generated by a thruster magnetic circuit. In the most general form, the motion of ions and neutrals is described by a system of kinetic equations for the distribution function  $f_k(t, \vec{x}, \vec{v})$  of the  $k$ th species with a charge  $Z_k$  (in electron charges  $e$ ) and mass  $m_k$ :

$$\frac{\partial f_k}{\partial t} + \vec{v} \frac{\partial f_k}{\partial \vec{x}} + \frac{eZ_k}{m_k} \left( \vec{E} + \frac{1}{c} [\vec{v} \times \vec{B}] \right) \frac{\partial f_k}{\partial \vec{v}} = St_k,$$

where  $St_k$  is the collision integral.

The distribution of the potential  $\phi$  of the electric field  $\vec{E} = -\vec{\nabla}\phi$  is determined from the solution of the Poisson equation

$$\Delta\phi = 4\pi e \left( n_e - \sum_k Z_k n_k \right),$$

where  $n_e$  and  $n_k$  are the number densities of electrons and ions of the  $k$ th species.

There are some important factors that affect simulation of ions and neutrals.

1. The gyro radius of ions is much greater than the size of interest; hence, the influence of the magnetic field on ion motion may be ignored.
2. The influence of ions and neutrals produced by sputtering of thruster walls on the remaining components of the plume may be ignored because of the comparatively low concentration of the former.
3. The densities of components and the cross sections of collisional processes are such that only elastic and CEX ion-neutral collisions have a significant effect on the distribution functions of ions and neutrals.

Determination of the distribution function of electrons is the most complicated part of thruster simulation. In the present work, the simplest model of isothermal electrons, which are described by the Boltzmann distribution:

$$n_e(\vec{x}) = n_e^0 \exp \left( \frac{e\phi(\vec{x})}{kT_e} \right),$$

is used.  $T_e$  is the temperature of electrons,  $k$  is the Boltzmann constant, and  $n_e^0$  is the value of the electron number density for  $\phi = 0$ .

The Debye radius of electrons  $R_d = \sqrt{T_e/4\pi e^2 n_e}$  in the SPT plume plasma is much smaller than the other characteristic dimensions. Hence, the condition of quasi-neutrality  $n_e = \sum_k Z_k n_k$  may be used, where  $n_k$  is the number density of various kinds of ions. Then the electric potential is found directly from the ion number density

$$\phi(\vec{x}) = \frac{kT_e}{e} \ln \left( \frac{1}{n_e^0} \sum_k Z_k n_k(\vec{x}) \right),$$

instead of solving the Poisson's equation.

Thus, simulation of the SPT plume plasma reduces to solving, by the Monte Carlo method, kinetic equations for ions and neutrals. Collisions between charged particles are ignored, and the effect of the magnetic field on ion motion is assumed to be insignificant.

The electric potential is determined directly from the ion number density using the quasi-neutrality assumption or numerically solving the Poisson's equation. In the numerical methods described below, both variants of potential calculation were used, though the calculation results show that the difference was observed only in a very thin sheath near the thruster walls.

## COMPUTATIONAL METHODS

Numerical simulation of the SPT thruster plume on the basis of the model presented in the previous section was performed using two methods: combinations of the particle-in-cell method with the direct simulation Monte Carlo method (PIC-DSMC) and the particle-in-cell with the addition of Monte Carlo collisions method (PIC-MCC). The difference in these methods refers primarily to the description of collisional processes in plasma. The dynamics of ions in both methods are simulated identically.

The main specific features are briefly described below.

1) PIC-DSMC (combination of PIC and DSMC).

In this method, ion and neutral flows are simulated simultaneously. The motion of ions is calculated by PIC method at each time step, while the motion of neutrals is calculated by DSMC method. All collisions (neutral-neutral and ion-neutral) are simulated by the DSMC method.

The main feature of the PIC-DSMC method for simulation of the SPT thruster plume is taking into consideration the influence of ion-neutral collisions on the distribution function of neutrals.

2) PIC-MCC.

The use of this method for solving the problem posed is based on the assumption that the influence of ion-neutral collisions on the neutral distribution function is insignificant. Thus, the problem is divided into two stages:

- first stage - computation of density, temperature and velocity of propellant and ambient neutrals by the DSMC method, and
- second stage - PIC-MCC computations of the flow of charged species of the plume using DSMC flowfields of neutrals for simulation of ion-neutral collisions.

The main advantage of the PIC-MCC method is its significant computational economy as compared to the PIC-DSMC method, because the PIC-MCC method does not require simultaneous simulation of ions and neutrals.

## FLOW CONDITIONS

Propellant ions: singly  $Xe^+$  and doubly charged  $Xe^{++}$  and neutrals  $Xe$  flow out from an annular exit of the SPT-100 thruster with a 28-mm inner diameter and a 50-mm outer diameter. A hollow cathode, which is a source of electrons, is located behind the thruster exit plane to the side of the thruster. In addition, the cathode emits neutrals with roughly identical parameters as the propellant neutrals issued from the thruster. The fraction of neutrals from the cathode is characterized by the magnitude of cathode split and usually amounts to  $\sim 10\%$  of the total mass flow rate.

To simplify the simulation, we assume that the flow is axisymmetric around the thruster centerline. Therefore, the cathode is not represented explicitly in simulations, and it is assumed that cathode neutrals leave the thruster exit, as propellant neutrals do [4].

The computational domain is a rectangle with the following dimensions: the lower boundary coincides with the axis of symmetry, the upper boundary is 0.6 m from the axis, the left boundary is located 0.3 m upstream of the thruster exit plane, and the right boundary is 0.6 m downstream of the thruster exit plane.

In this work, the SPT-100 thruster is simulated under the following operating conditions: discharge voltage 300 V, discharge current 4.5 A, and total mass flow rate 5.2 mg/s. The flow parameters at the thruster exit are determined by analysis and evaluation using the measured properties of the thruster such as the mass flow rate, ionization efficiency, etc. The use of different assumptions and data acquisition methods leads to somewhat different flow conditions at the thruster exit. To study the effect of these conditions on the plume structure and especially backflow, the following set of flow conditions was used in this work.

**Case 1.** The conditions of [3] were accepted as the basic case. This case corresponds to the following parameters: average energy of singly charged ions 300 eV (corresponding velocity 21,000 m/s), average energy of doubly charged ions 600 eV (29,700 m/s), double ion fraction 25%, ionization efficiency  $\eta_i = 96\%$ , cathode split  $\eta_s = 7\%$ , and ion temperature  $T_i = 4$  eV. The divergence angle of the ion velocity is assumed to vary linearly from -10 degrees to 10 degrees from the centerline with increasing of the radial position.

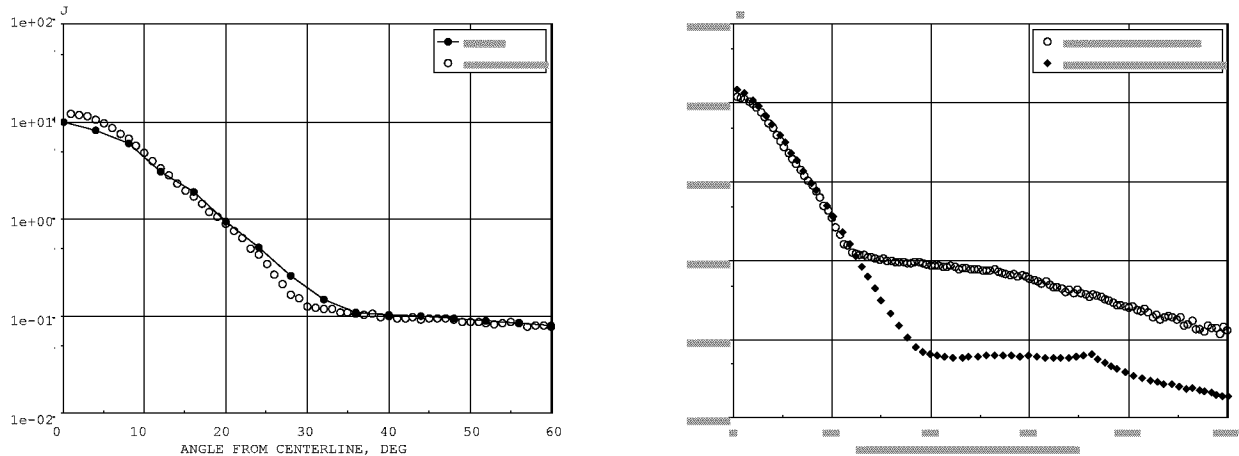
The velocity of the neutrals is assumed to be equal to the velocity of sound based on the stagnation temperature  $T_0 = 1000$  K. The density of ions and neutrals was assumed to be uniform over the exit plane. The electron temperature was assumed to be equal to 3 eV.

**Case 2.** As was shown in the experiments [6], the electron temperature in the near vicinity of the thruster exit reaches  $\sim 10$  eV. In the far field of the thruster plume, it is considerably smaller and close to  $T_e \sim 1$  eV. Therefore, an electron temperature  $T_e = 1$  eV was used to analyze the influence of the electron temperature in this test case. All the remaining parameters are equal to the corresponding parameters of case 1.

**Case 3.** The data reported by different authors on the scatter in the velocity of propellant ions at the thruster exit, which is characterized by the ion temperature, significantly varies. For example, the Maxwell velocity distribution for sampling of ion velocities with different values of temperature in the axial, radial and circumferential directions was used in [2]:  $T_x = 3.4$  eV,  $T_y = 0.7$  eV,  $T_z = 0.07$  eV. To estimate the ion temperature effects on the flow structure, computations with different ion temperatures in different directions were conducted.

**Case 4.** Some of experimental data [6] yield the double ion fraction  $\eta_d \sim 10\%$ , which is less than the value used in case 1. For a fixed value of the total mass flow rate and ionization efficiency, the energy of the directed motion of propellant ions is 225 eV for singly charged ions and 450 eV for doubly charged ions.

**Case 5.** According to measurements from NASA's Lewis Research Center [7], the beam divergence angle can vary from -27 to +41 deg with increasing radial position. The value of the double ion fraction is the same as for case 4.



**FIGURE 1.** Ion current density at a radial distance of 50 cm. Comparison with results of [3] (left). Influence of the ambient gas (right). Pressure of the ambient gas is 6 mPa.

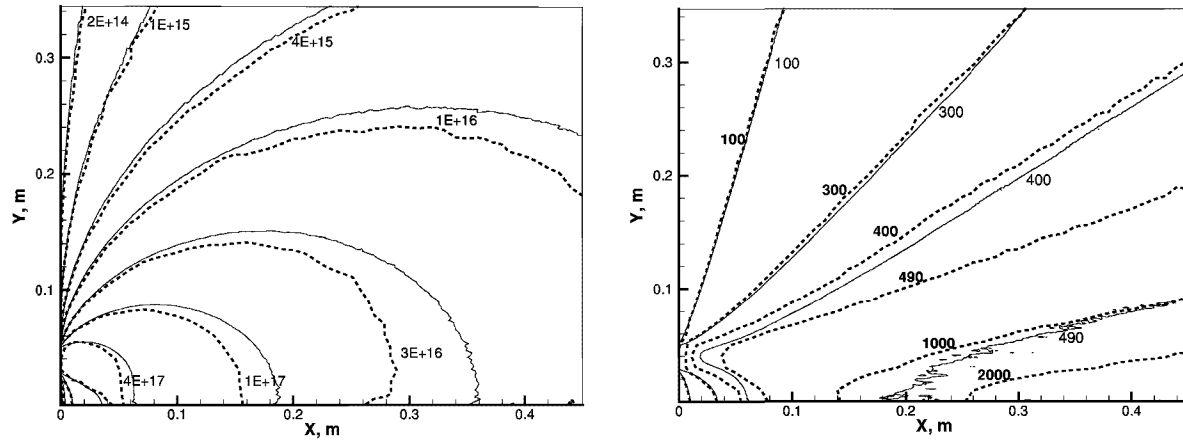
## RESULTS

Two codes based on the PIC-MCC and PIC-DSMC methods were developed. Comparison with numerical results of [3] is illustrated in Fig. 1, which shows the calculated angular distribution of the ion current density under conditions corresponding to case 1. It is seen that PIC-MCC results and the PIC-DSMC results of [3] are in good agreement. Hence, the use of the PIC-MCC method for simulating SPT plumes taking into account the ambient gas allows one to obtain results with a reasonable accuracy rather fast.

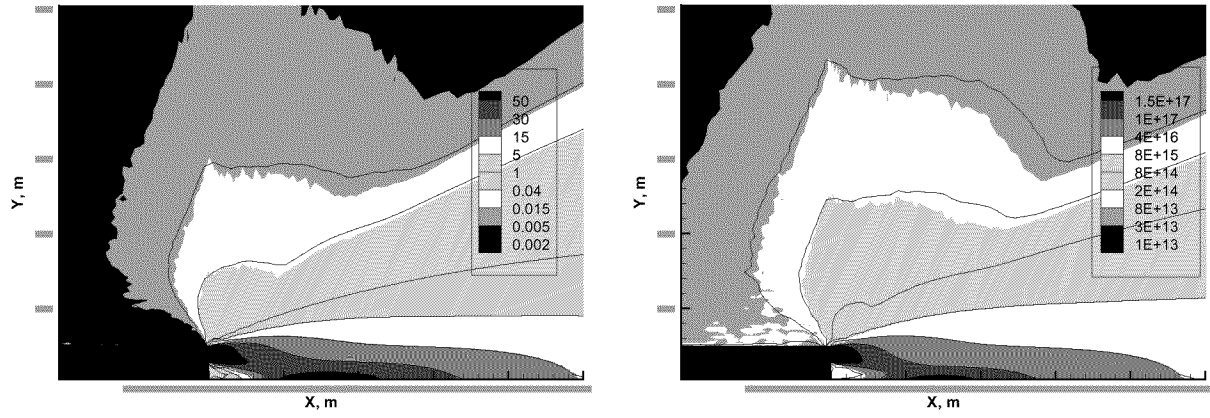
Figure 1 also shows the ambient gas effect on the angular distribution of the ion current density for case 1. These calculations were performed by the PIC-MCC method. The effect of the ambient gas on CEX ion backflow (the angle from the centerline is more than 50 deg) is rather significant (the difference reaches more than an order of magnitude). The reason is that the density of propellant neutrals at the thruster exit plane and the ambient gas density have close values; however, the density of propellant neutrals dramatically decreases with distance from the exit plane, whereas the ambient gas density is constant.

Therefore, a correct prediction of CEX ion backflow at conditions of space flight requires a computational study of the thruster plume flow without the ambient gas. Simulation of the ion backflow by the PIC-DSMC method involves large computer resources than the PIC-MCC method even in the absence of the ambient gas. To clarify the applicability of the PIC-MCC method in the case where the CEX ion backflow is formed only due to the collisions of fast ions with propellant neutrals, it is necessary to analyze the influence of these collisions on neutrals of the SPT thruster plume.

First consider a detailed comparison of the PIC-MCC and PIC-DSMC methods for case 1. The fields of the number density of neutrals obtained with the help of these methods are plotted in Fig. 2. It is clearly seen that the PIC-MCC method predicts a somewhat higher value of density than PIC-DSMC within the entire flow field. The reason is that taking into account ion-neutral collisions in PIC-DSMC leads to a significantly greater value of the neutral velocity, which leads to a lower density for a fixed total flow rate of the propellant. Figure 2 also shows the fields of the axial component of the neutral velocity. In the region adjacent to the axis, at a distance of 0.2–0.5 m from the thruster, the mean axial velocity obtained by the PIC-MCC method lies within 490–550 m/s. The PIC-DSMC calculation shows that the axial velocity of neutrals in this region is greater than 1000 m/s and increases to 2000 m/s downstream. At the same time, the isolines of the axial component of velocity almost coincide far from the axis (see Fig. 2). This is explained by the fact that fast (CEX) neutrals are almost absent there. They are mainly formed in the region adjacent to the thruster exit and move in the same direction as fast ions, i.e., mainly along the axis. Thus, the influence of ion-neutral collisions leads to an increase in the axial component of neutral velocity and, hence, to a lower density as compared to the result obtained using the PIC-MCC method with ignored effect of ions on neutrals.

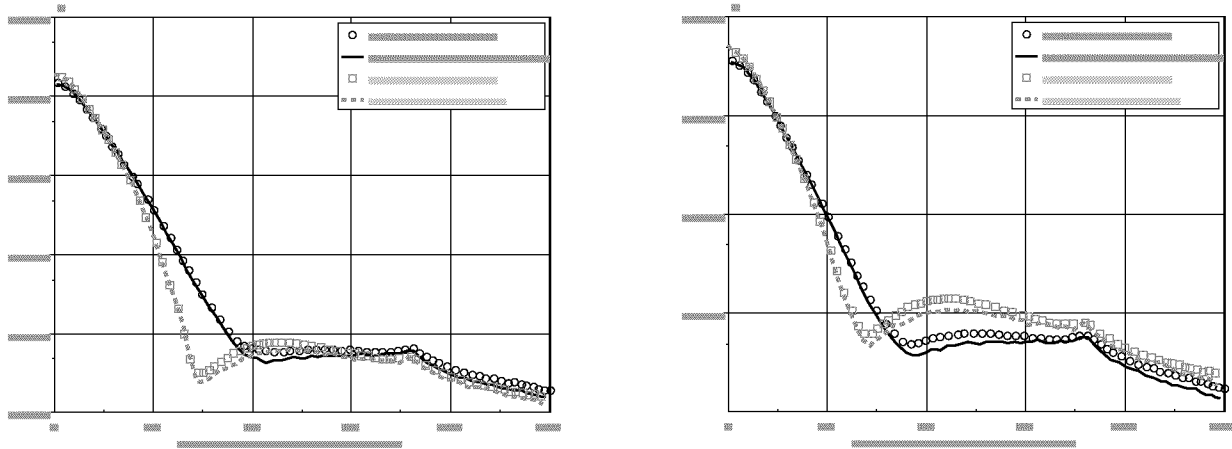


**FIGURE 2.** Number density of neutrals (left),  $\text{\#/m}^3$ , and axial velocity of neutrals (right),  $\text{m/s}$  (PIC-MCC - solid lines, PIC-DSMC - dashed lines).



**FIGURE 3.** Ion current density (left),  $\text{mA}/\text{cm}^2$ , and number density of electrons (right),  $\#/\text{m}^3$ , (PIC-MCC - lines, PIC-DSMC - flood).

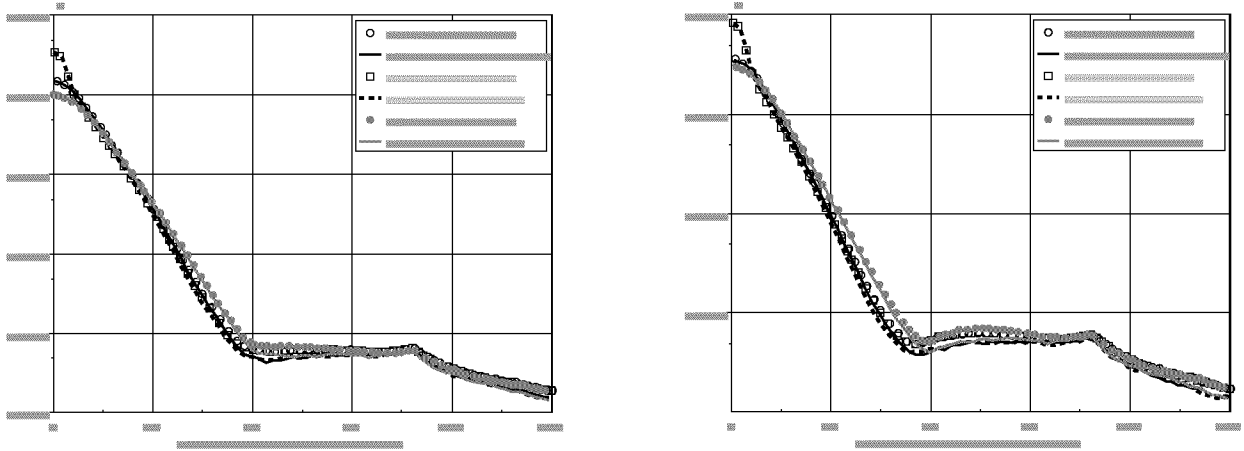
Figure 3 shows the fields of the ion current density and electron number density. Because of the quasi-neutrality of the plasma, the latter is equal to  $n_1 + n_2$ , where  $n_1$  and  $n_2$  are the number densities of singly and doubly charged ions, almost within the entire flow region except for a thin sheath near the thruster walls. In the plume core, the results obtained by the PIC-MCC and PIC-DSMC methods coincide. Some difference is observed in the backflow region, which is manifested in a greater value of both the ion current density and the electron density predicted by the PIC-MCC method. This difference can be estimated qualitatively by the angular distribution of these quantities shown in Fig. 4. A noticeable difference between the results predicted by the two methods is observed within the range of angles from 40 to 80 degrees. The difference in the electron density is slightly greater than in the ion current density and reaches the maximum value (25 %) for 50 deg.



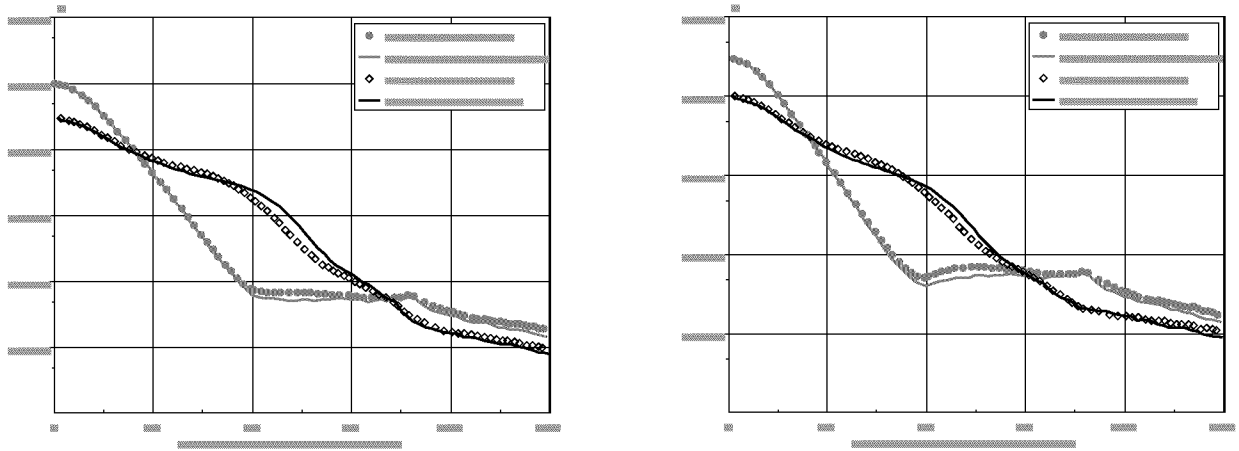
**FIGURE 4.** Ion current density (left),  $\text{mA}/\text{cm}^2$ , and electron number density (right),  $\#/\text{m}^3$ , at a radial distance of 50 cm.

Figure 4 also shows the curves of the ion current density and electron number density obtained by PIC-MCC and PIC-DSMC calculations for case 2. A decrease in the electron temperature leads to a smaller divergence of the central part of the plume: the angular width of the central part is 50 and 40 deg for  $T_e = 3 \text{ eV}$  and  $T_e = 1 \text{ eV}$ , respectively. It is of interest to note that the difference in the magnitude of the current density in the peripheral region of the plume lies within 25% for the considered values of the electron temperature, and the number density is almost two times higher for case 2.

The effect of the ion temperature on the angular distribution of the ion current density and electron number density is illustrated in Fig. 5. A significant decrease in the ion temperature in the radial and circumferential directions affects the flow only near the centerline. The magnitude of the current and number density increases more than a factor of 2 as compared to the values for case 1. Note that the difference between PIC-MCC and PIC-DSMC predictions for case 3 is also within 25%, which is significantly smaller than the ion temperature effect. A decrease in the double ion fraction and ion velocity at the thruster exit leads to a somewhat greater divergence of the central part of the plume and to a small decrease in the current and density values on the centerline (see the curves for case 4 in Fig. 5)



**FIGURE 5.** Ion current density (left),  $\text{mA}/\text{cm}^2$ , and electron number density (right),  $\#/\text{m}^3$ , at a radial distance of 50 cm.



**FIGURE 6.** Ion current density (left),  $\text{mA}/\text{cm}^2$ , and electron number density (right),  $\#/\text{m}^3$ , at a radial distance of 50 cm.

Figure 6 shows a comparison of results obtained for case 4 and case 5. The difference in the current density is quite significant. Within the range of angles from 25 to 80 deg, the values of the current density and density obtained in calculations for case 4 are much greater than the corresponding values for case 5. For example, in the vicinity of 50 deg, the difference is more than an order of magnitude. At the same time, within the range of angles from 0 to 20 deg, vice versa, the values for case 4 are greater than for case 5; in particular, there is more than a threefold difference between them at the centerline. It is of interest that an increase in the divergence

angle leads to a decrease in the current and density in the backflow region. For angles greater than 90 deg, the values for case 4 are greater than those for case 5 by more than a factor of 2.

The results presented demonstrate that the difference between the values of the ion current density and electron density obtained by the PIC-MCC and PIC-DSMC methods does not exceed 30%, which is considerably smaller than the effect of the thruster exit conditions (especially, the divergence angle).

## CONCLUSIONS

Two codes based on two methods (PIC-MCC and PIC-DSMC) for the modeling of the SPT-100 thruster plume have been developed. The main difference between these methods is that the PIC-DSMC method takes into account the influence of ion-neutral collisions on neutrals. The analysis shows that the greatest difference in results obtained by both methods is observed in the neutral velocity near the centerline. At the same time, the difference in the ion current density and electron number density is less than 25%.

The boundary conditions at the thruster exit plane are not well-defined for the SPT-100. A series of computations with different thruster exit conditions was performed to reveal the effect of these conditions. The effect of the electron temperature on the plume flow is significant in the central part of the plume. The change in the electron temperature from 3 eV to 1 eV decreases the divergence of the plume core from 50 to 40 deg. The values of the ion current density in the backflow region differ by less than 25%, and the value of the electron density obtained using  $T_e = 1$  eV is almost two times smaller.

A decrease in the temperature of propellant ions in the radial and circumferential directions leads to an increase in the electron density and ion current density in the region adjacent to the thruster centerline by more than a factor of 2 and does not exert a significant effect on the backflow. A decrease in the double ion fraction and ion velocity at the thruster exit leads to a moderate divergence of the core plume and has practically no effect on the backflow. The divergence angle exerts the greatest effect on the plume structure as a whole, including a more than twofold increase in the ion backflow current.

The analysis shows that the influence of uncertainties in flow parameters at the SPT-100 thruster exit is much greater than the difference in results obtained by the PIC-MCC and PIC-DSMC methods. Thus, with current uncertainties in formulation of the boundary conditions, the use of a simpler and more economical (from the computational viewpoint) PIC-MCC method in the axisymmetric case yields results with an identical accuracy as the PIC-DSMC method.

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